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EXTINCTION AND POLARIZATION OF TRANSMITTED LIGHT BY PARTIALLY ALIGNED NONSPHERICAL GRAINS

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ABSTRACT

The problem of model theoretical calculation of the interstellar extinction and polarization due to nonspherical grains partially aligned in a magnetic field is considered. The Waterman's T-matrix approach is used to develop a rigorous analytical method to average the extinction matrix over orientations of a nonspherical grain. The method results in minimizing the numerical effort and can be used for efficient numerical calculations in the resonance region of grain size parameters.

Numerical aspects of the proposed method are discussed in detail. The range of validity of the Rayleigh approximation in calculating the extinction matrix for partially aligned spheroidal grains is examined, i.e., the values of the equal-volume–sphere size parameter are determined below which the Rayleigh-limit formulae are accurate within a given error.

Subject headings: interstellar: grains — polarization – radiative transfer

I. INTRODUCTION

Interstellar extinction and linear and circular polarization serve as an important source of our information concerning the properties of interstellar dust grains. To infer the size, morphology, and composition of the interstellar grains, one should compare observations of the interstellar extinction and polarization, on the one hand, and model computations, on the other. Therefore, the results of interpreting the observational data greatly depend upon our ability to theoretically calculate the extinction and polarization of transmitted light due to partially aligned nonspherical grains of realistic shape. According to Mathis, Rumpl, and Nordsieck (1977), Hong and Greenberg (1980), Aannestad and Greenberg (1983), Draine and Lee (1984), Lee and Draine (1985), Chlewicki and Laureijs (1988), Duley, Jones, and Williams (1989), interstellar grains have a range of sizes extending up to a few tenths of micrometer. Thus, in interpreting the observations in the ultraviolet and visual regions, theoretical calculations for the so-called resonance particles (i.e., for particles with sizes of the order of wavelength) are of particular importance.

Theoretical computations for partially aligned resonance nonspherical particles of realistic shape are very complicated, the numerical averaging of the scattering properties of a nonspherical grain over its orientations being the most time-consuming step (see, e.g., Rogers and Martin 1979; Wiscombe and Mugnai 1986). Therefore, to minimize the numerical effort, it is highly desirable to develop an exact analytical averaging method rather than to use the common numerical averaging procedure.

Recently, several approaches have been developed to compute scattering properties of a single resonance nonspherical particle with a fixed orientation. Oguchi (1973), Asano and Yamamoto (1975), Onaka (1980), and Farafonov (1983) used separation of variables in a spheroidal coordinate system to solve the scattering problem for homogeneous and layered spheroids. Purcell and Pennypacker (1973) have proposed the so-called discrete-dipole method to compute scattering by a particle of arbitrary shape; in particular, the discrete-dipole method is applicable to particles composed of optically anisotropic materials (see also Yung 1978; Chiappetta, Perrin, and Torresani 1987; Draine 1988; Singham and Bohren 1989). Waterman (1965, 1971) has developed the T-matrix method (or extended boundary condition method) which can be used in calculations for arbitrarily shaped particles, although it was mainly applied to axially symmetric objects (see also Ström 1975; Barber and Yeh 1975; Waterman 1979; Varadan and Varadan 1980). Holt, Uzunoglu, and Evans (1978) and Shepherd and Holt (1983) have used the method of Fredholm integral equation to calculate scattering properties of ellipsoids and finite cylinders. More thorough reviews and comparisons of the available methods may be found in Oguchi (1981), Holt (1982), Barber and Massoudi (1982), Mon (1982), and Wiscombe and Mugnai (1986).

Comparative analysis of the relevant literature shows that, in application to axially symmetric particles consisting of optically isotropic materials, the T-matrix approach seems to be the most efficient and to be used in a greater range of scattering problems. Computations were reported for homogeneous and layered particles of different shape: oblate and prolate spheroids (up to very high aspect ratios), finite cylinders, Chebyshev particles, and particles with axisymmetric surface perturbations (see, e.g., Peterson and Ström 1974; Warner and Hizal 1976; Bringi and Seliga 1977; Wang and Barber 1979; Mugnai and Wiscombe 1980; Lakhtakia, Varadan, and Varadan 1984; Geller, Tsuei, and Barber 1985; Wiscombe and Mugnai 1986). However, the main advantage of the T-matrix approach is the analyticity of its mathematical formulation, which permits a deeper insight into the essence of wave scattering (Varadan and Varadan 1980). In particular, the T-matrix approach is ideally suited for analytical averaging of the scattering properties of a nonspherical grain over its orientations (Varadan 1980; Tsang, Kong, and Shin 1984; Mishchenko 1990).

In the present paper, we study the problem of theoretical calculation of the extinction, linear and circular polarization of transmitted light by nonspherical grains partially aligned in a magnetic field. Specifically, the T-matrix approach is used to develop an exact analytical method to average the extinction matrix over orientations of a nonspherical grain. We assume here that, whatever the actual physical mechanism of grain alignment is, the distribution of dust particles over orientations is axially aymmetric, the direction of the local magnetic field being the axis of symmetry (see, e.g., Martin 1978; Dolginov, Gnedin, and Silant'ev 1979).

The plan of our paper is as follows. In § II, the problem of calculating the extinction and polarization of light transmitted by a slab of partially aligned nonspherical grains is mathematically formulated. In § III, an analytical method for calculating the orientationally averaged extinction matrix is described. In § IV, some numerical aspects of the proposed method are discussed, and several illustrative numerical results are presented. In § V, the range of validity of the Rayleigh approximation in calculating the orientationally averaged extinction matrix is examined. Finally, in § VI, the principal results of the paper are summarized.

II. RADIATIVE TRANSFER EQUATION

To describe the scattering of polarized light in some scattering medium, we use a right-handed Cartesian coordinate system $B = OXYZ$ with orientation fixed in space, having its origin O inside a single scattering particle (§ II*a*), or inside a small volume element (§ II*c*). In what follows, this coordinate system will be referred to as the laboratory reference frame.

The direction of a beam of light is specified by a unit vector $\boldsymbol{n} = (\theta, \varphi)$, where θ $(0 \leq \theta \leq \pi)$ is a zenith angle measured from the positive z-axis, and $\varphi (0 \leq \varphi \leq 2\pi)$ is an azimuth angle measured from the positive x-axis in the clockwise sense, when looking in the direction of the positive z-axis.

θ- and φ-components of the electric field $\boldsymbol{E}$ are supplied by subscripts 1 and 2, respectively. Thus, the component $\boldsymbol{E}_1 = E_1 \hat{\boldsymbol{\theta}}$ is along the meridional plane (plane through the beam and the z-axis), whereas the component $\boldsymbol{E}_2 = E_2 \hat{\boldsymbol{\varphi}}$ is perpendicular to this plane; here, $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\varphi}}$ are the corresponding unit vectors (note that $\boldsymbol{n} = \hat{\boldsymbol{\theta}} \times \hat{\boldsymbol{\varphi}}$).

a) Single Scattering

Consider a plane electromagnetic wave

$$\begin{aligned} \boldsymbol{E}^i(\boldsymbol{r}) &= (\boldsymbol{E}_1^i + \boldsymbol{E}_2^i) \exp(ik\boldsymbol{n}_i \boldsymbol{r}) \\ &= (E_1^i \hat{\boldsymbol{\theta}}_i + E_2^i \hat{\boldsymbol{\varphi}}_i) \exp(ik\boldsymbol{n}_i \boldsymbol{r}) , \end{aligned} \tag{2.1}$$

incident upon a nonspherical particle; here, $k = 2\pi/\lambda$, and λ is a free-space wavelength. The time factor $\exp(-i\omega t)$ is assumed and suppressed throughout the paper. In the far-field zone ($kr \gg 1$), the scattered wave becomes spherical and is given by (see van de Hulst 1957; Bohren and Huffman 1983)

$$\begin{gathered} \boldsymbol{E}^s(\boldsymbol{r}) = E_1^s(r, \boldsymbol{n}_s)\hat{\boldsymbol{\theta}}_s + E_2^s(r, \boldsymbol{n}_s)\hat{\boldsymbol{\varphi}}_s , \qquad \boldsymbol{n}_s = \boldsymbol{r}/r , \\ \boldsymbol{E}^s(\boldsymbol{r}) \cdot \boldsymbol{r} = 0 , \\ \begin{bmatrix} E_1^s \\ E_2^s \end{bmatrix} = \frac{\exp(ikr)}{r} \boldsymbol{F}(\boldsymbol{n}_s, \boldsymbol{n}_i) \begin{bmatrix} E_1^i \\ E_2^i \end{bmatrix} , \end{gathered} \tag{2.2}$$

where $\boldsymbol{F}$ is a (2×2) amplitude scattering matrix. This matrix depends (besides $\boldsymbol{n}_i$ and $\boldsymbol{n}_s$) upon the size, morphology, and composition of the scattering particle, as well as on its orientation with respect to the laboratory reference frame B.

As was shown by Saxon (1955), the amplitude scattering matrix obeys a reciprocity relation

$$\boldsymbol{F}(\boldsymbol{n}_s, \boldsymbol{n}_i) = \boldsymbol{Q}\boldsymbol{F}^T(-\boldsymbol{n}_i, -\boldsymbol{n}_s)\boldsymbol{Q} , \tag{2.3}$$

where $\boldsymbol{Q} = \mathrm{diag}(1, -1)$, and T denotes matrix transposition.

b) Stokes Parameters

In this paper, we use the Stokes parameters of the incident and scattered waves defined as

$$\begin{aligned} I &= E_1 E_1^* + E_2 E_2^* , \\ Q &= E_1 E_1^* - E_2 E_2^* , \\ U &= E_1 E_2^* + E_2 E_1^* , \\ V &= i(E_1 E_2^* - E_2 E_1^*) , \end{aligned} \tag{2.4}$$

where the asterisk denotes the conjugate complex value (for extensive discussion of polarimetric definitions see, e.g., Clarke 1974*a*, *b*; Hovenier and van der Mee 1983). Further, the Stokes vector $\boldsymbol{I}$ is defined as a (4×1) column having the Stokes parameters as its components as follows:

$$\boldsymbol{I} = (I, Q, U, V)^T = \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} . \tag{2.5}$$

c) *The Equation of Transfer*

The Stokes vector of radiation in a sparse medium, consisting of randomly positioned discrete scatterers, obeys the radiative transfer equation (see, e.g., Rozenberg 1955; Dolginov, Gnedin, and Silant'ev 1970; Ishimaru and Yeh 1984)

$$\begin{aligned} n\nabla_R I(R, n) &= dI(R, n)/ds \\ &= n_d(R)K(R, n)I(R, n) + n_d(R)\int_{4\pi} dn' Z(R, n, n')I(R, n') , \end{aligned} \quad (2.6)$$

where the pathlength element ds is measured along the unit vector n, $n_d(R)$ is the number density of dust particles at a point R, $K(R, n)$ is a (4×4) extinction matrix, and $Z(R, n, n')$ is a (4×4) phase matrix. Let n be the direction of incidence of light upon a slab of dust grains. In model theoretical computations of the interstellar extinction and polarization, one is interested in calculating only the Stokes parameters of unscattered light transmitted by the slab. Therefore, the second term on the right-hand side of equation (2.6), which describes effects of multiple scattering of light, can be omitted, and the radiative transfer equation to be solved becomes

$$dI(R, n)/ds = n_d(R)K(R, n)I(R, n) . \quad (2.7)$$

The elements of the extinction matrix are expressed in the elements of the forward-scattering amplitude matrix as follows (Dolginov, Gnedin, and Silant'ev 1979; Ishimaru and Yeh 1984):

$$\begin{aligned} K_{jj}(R, n) &= -\frac{2\pi}{k}\,\mathrm{Im}\,[\langle F_{11}(R, n, n)\rangle + \langle F_{22}(R, n, n)\rangle] , \qquad j = 1, \dots, 4 , \\ K_{12}(R, n) &= K_{21}(R, n) = \frac{2\pi}{k}\,\mathrm{Im}\,[\langle F_{22}(R, n, n)\rangle - \langle F_{11}(R, n, n)\rangle] , \\ K_{13}(R, n) &= K_{31}(R, n) = -\frac{2\pi}{k}\,\mathrm{Im}\,[\langle F_{12}(R, n, n)\rangle + \langle F_{21}(R, n, n)\rangle] , \\ K_{14}(R, n) &= K_{41}(R, n) = \frac{2\pi}{k}\,\mathrm{Re}\,[\langle F_{21}(R, n, n)\rangle - \langle F_{12}(R, n, n)\rangle] , \\ K_{23}(R, n) &= -K_{32}(R, n) = \frac{2\pi}{k}\,\mathrm{Im}\,[\langle F_{21}(R, n, n)\rangle - \langle F_{12}(R, n, n)\rangle] , \\ K_{24}(R, n) &= -K_{42}(R, n) = -\frac{2\pi}{k}\,\mathrm{Re}\,[\langle F_{12}(R, n, n)\rangle + \langle F_{21}(R, n, n)\rangle] , \\ K_{34}(R, n) &= -K_{43}(R, n) = \frac{2\pi}{k}\,\mathrm{Re}\,[\langle F_{11}(R, n, n)\rangle - \langle F_{22}(R, n, n)\rangle] , \end{aligned} \quad (2.8)$$

where angle brackets denote an average over orientations of the scattering grains.[1]

From the definition (2.8) and equation (2.3), we easily derive the reciprocity relation for the extinction matrix,

$$K(R, n) = PK^T(R, -n)P , \quad (2.9)$$

where $P = \mathrm{diag}\,(1, 1, -1, 1)$.

Numerical solution of equation (2.7) usually presents no difficulties. The main problem is to calculate the orientationally averaged extinction matrix for an ensemble of partially aligned nonspherical grains. In the next section, we shall describe an efficient analytical method for calculating the extinction matrix for nonspherical grains partially aligned in a magnetic field. Thus, it will be assumed that the angular momentum J of a spinning grain is perfectly aligned with the principal axis of the largest momentum of inertia, and J processes around the vector B of the local magnetic field (Purcell 1979). In § III*a*, the magnetic field B will be assumed to be parallel to the z-axis of the laboratory reference frame. Then, in § III*b*, the general case $B \nparallel OZ$ will be considered.

III. CALCULATION OF THE EXTINCTION MATRIX FOR NONSPHERICAL GRAINS PARTIALLY ALIGNED IN A MAGNETIC FIELD

a) $B \parallel OZ$

For calculating the elements of the amplitude scattering matrix $F(n_s, n_i)$ for a nonspherical grain with a fixed orientation, we use the T-matrix approach (Waterman 1971). We expand the incident and scattered fields in vector spherical waves (see Appendix A) as follows:

$$E^i(r) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} [a_{mn}\,\mathrm{Rg}\,M_{mn}(kr) + b_{mn}\,\mathrm{Rg}\,N_{mn}(kr)] , \quad (3.1)$$

$$E^s(r) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} [p_{mn} M_{mn}(kr) + q_{mn} N_{mn}(kr)] , \qquad r > r_0 , \quad (3.2)$$

[1] Note that in calculating the ensemble averages, we should also take into account distribution of the scattering grains over sizes, shapes, refractive indices, etc. This can be done by straightforward averaging procedures and will not be discussed in this paper.

where r_0 is the radius of a circumscribing sphere of the scattering grain. Due to linearity of Maxwell equations, the relation between the scattered field coefficients and exciting field coefficients is linear and is given by a transition matrix (or the T-matrix) $\boldsymbol{T}$ as follows:

$$p_{mn} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} [T^{11}_{mnm'n'} a_{m'n'} + T^{12}_{mnm'n'} b_{m'n'}] , \tag{3.3}$$

$$q_{mn} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} [T^{21}_{mnm'n'} a_{m'n'} + T^{22}_{mnm'n'} b_{m'n'}] . \tag{3.4}$$

By use of a compact notation, we also write

$$\begin{bmatrix} p \\ q \end{bmatrix} = T \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} T^{11} & T^{12} \\ T^{21} & T^{22} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} . \tag{3.5}$$

The elements of the T-matrix do not depend upon the directions of propagation and the states of polarization of the incident and scattered fields. They depend only upon the size, morphology, and composition of the scattering grain, and on its orientation with respect to the laboratory reference frame.

For a plane incident wave

$$\boldsymbol{E}^i(\boldsymbol{r}) = \boldsymbol{E}_i \exp (ik\boldsymbol{n}_i \boldsymbol{r}) , \tag{3.6}$$

the expansion coefficients are (Tsang, Kong, and Shin 1984)

$$a_{mn} = 4\pi(-1)^m i^n d_n \boldsymbol{C}^*_{mn}(\theta_i)\boldsymbol{E}_i \exp (-im\varphi_i) , \tag{3.7}$$

$$b_{mn} = 4\pi(-1)^m i^{n-1} d_n \boldsymbol{B}^*_{mn}(\theta_i)\boldsymbol{E}_i \exp (-im\varphi_i) \tag{3.8}$$

(see definitions [A5], [A6], and [A8] of Appendix A). By making use of the large argument approximation for spherical Hankel functions

$$h_n^{(1)}(kr) \simeq \frac{(-i)^n \exp (ikr)}{ikr} , \qquad kr \gg n^2 , \tag{3.9}$$

and taking into account equations (2.2), (3.2)–(3.4), (3.7)–(3.8), and (A2)–(A3), we obtain an expression of the amplitude scattering matrix $\boldsymbol{F}$ in terms of the T-matrix elements (Waterman 1971; Tsang, Kong, and Shin 1984). In dyadic notations we have

$$\boldsymbol{F}(\boldsymbol{n}_s, \boldsymbol{n}_i) = \frac{4\pi}{k} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \sum_{m=-n}^{n} \sum_{m'=-n'}^{n'} i^{n'-n-1}(-1)^{m-m'} d_n d_{n'} \exp [i(m\varphi_s - m'\varphi_i)]$$
$$\times \left\{[T^{11}_{mnm'n'} \boldsymbol{C}_{mn}(\theta_s) + T^{21}_{mnm'n'} i\boldsymbol{B}_{mn}(\theta_s)]\boldsymbol{C}^*_{m'n'}(\theta_i) + [T^{12}_{mnm'n'} \boldsymbol{C}_{mn}(\theta_s) + T^{22}_{mnm'n'} i\boldsymbol{B}_{mn}(\theta_s)] \frac{\boldsymbol{B}^*_{m'n'}(\theta_i)}{i}\right\} . \tag{3.10}$$

To use equations (2.8) and (3.10) to calculate the orientationally averaged extinction matrix, we are to average the T-matrix elements over all grain orientations. Let a right-handed coordinate system A be attached fixedly to the scattering grain. This coordinate system will be referred to as the natural reference frame of the scatterer. Grain orientation with respect to the laboratory reference frame B we define by the Eulerian angles of rotation α, β, and γ that transform the coordinate system B into the coordinate system A (cf. Varshalovich, Moskalev, and Khersonskij 1975). In that way, we can write

$$\langle T^{ij}_{mnm'n'} \rangle = \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin \beta \int_0^{2\pi} d\gamma \, T^{ij}_{mnm'n'}(B; \alpha, \beta, \gamma)P(\alpha, \beta, \gamma) , \qquad i, j = 1, 2 , \tag{3.11}$$

where $\boldsymbol{T}(B; \alpha, \beta, \gamma)$ is the T-matrix of the scatterer calculated with respect to the laboratory reference frame, and $P(\alpha, \beta, \gamma)$ is a probability density function normalized as

$$\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin \beta \int_0^{2\pi} d\gamma \, P(\alpha, \beta, \gamma) = 1 . \tag{3.12}$$

If the local magnetic field $\boldsymbol{B}$ is parallel to the z-axis of the laboratory coordinate system, then

$$P(\alpha, \beta, \gamma) = \frac{1}{4\pi^2} p(\beta) , \tag{3.13}$$

and the normalizing condition becomes

$$\int_0^{\pi} d\beta \sin \beta p(\beta) = 1 . \tag{3.14}$$

Let $T(A)$ be the T-matrix calculated with respect to the natural reference frame of the scatterer. By making use of the formula (Varshalovich, Moskalev, and Khersonskij 1975)

$$M_{mn}(kr, \theta_A, \varphi_A) = \sum_{m'=-n}^{n} D^n_{m'm}(\alpha, \beta, \gamma) M_{m'n}(kr, \theta_B, \varphi_B) , \tag{3.15}$$

where $D^n_{m'm}(\alpha, \beta, \gamma)$ are Wigner D-functions (see Appendix A), and similar relations for the functions N_{mn}, Rg M_{mn}, and Rg N_{mn}, and taking into account equations (3.1)–(3.4), we have (Varadan 1980; Tsang, Kong, and Shin 1984)

$$T^{ij}_{mnm'n'}(B; \alpha, \beta, \gamma) = \sum_{m_1=-n}^{n} \sum_{m_2=-n'}^{n'} D^{-1n'}_{m_2m'}(\alpha, \beta, \gamma) T^{ij}_{m_1nm_2n'}(A) D^n_{mm_1}(\alpha, \beta, \gamma) , \tag{3.16}$$

where

$$D^{-1n'}_{m_2m'}(\alpha, \beta, \gamma) = [D^{n'}_{m'm_2}(\alpha, \beta, \gamma)]^* = D^{n'}_{m_2m'}(-\gamma, -\beta, -\alpha) . \tag{3.17}$$

By inserting equation (3.16) into equation (3.11), and taking into account equations (3.13) and (A1), we derive

$$\langle T^{ij}_{mnm'n'} \rangle = \delta_{mm'} \sum_{m_1=-M}^{M} T^{ij}_{m_1nm_1n'}(A) \int_0^\pi d\beta \sin \beta p(\beta) d^n_{mm_1}(\beta) d^{n'}_{mm_1}(\beta) , \tag{3.18}$$

where $\delta_{mm'}$ is the Kronecker delta, and $M = \min(n, n')$. Finally, by use of the Clebsch-Gordan expansion (see, e.g., Varshalovich, Moskalev, and Khersonskij 1975)

$$d^n_{mm_1}(\beta) d^{n'}_{mm_1}(\beta) = (-1)^{m+m_1} \sum_{n_1=|n-n'|}^{n+n'} C^{n_1 0}_{nmn'-m} d^{n_1}_{00}(\beta) C^{n_1 0}_{nm_1n'-m_1} , \tag{3.19}$$

we obtain

$$\langle T^{ij}_{mnm'n'} \rangle = \delta_{mm'} T^{ij}_{mnn'} , \tag{3.20}$$

$$T^{ij}_{mnn'} = \sum_{m_1=-M}^{M} \sum_{n_1=|n-n'|}^{n+n'} (-1)^{m+m_1} p_{n_1} C^{n_1 0}_{nmn'-m} C^{n_1 0}_{nm_1n'-m_1} T^{ij}_{m_1nm_1n'}(A) , \tag{3.21}$$

where

$$p_n = \int_0^\pi d\beta \sin \beta p(\beta) d^n_{00}(\beta) . \tag{3.22}$$

In other words, the quantities p_n are coefficients in the expansion of the function $p(\beta)$ in Legendre polynomials (see eq. [A10])

$$p(\beta) = \sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(\cos \beta) p_n . \tag{3.23}$$

Thus, for calculating the orientationally averaged T-matrix $\langle T \rangle$, it is not necessary to calculate the integral in the right-hand side of equation (3.11) numerically by computing the matrix $T(B; \alpha, \beta, \gamma)$ for a great number of grain orientations. It is sufficient to calculate the matrix $T(A)$ once with respect to an arbitrarily chosen natural reference frame and then use equations (3.20) and (3.21).

As was mentioned above, at present the T-matrix approach is of practical use only for axially symmetric objects. Therefore, in what follows we shall assume that the scattering grains are axisymmetric, and the z-axis of the natural reference frame is the axis of symmetry. In that case, the formulae for calculating the matrix $T(A)$ become much simpler. In particular, it follows from these formulae that

$$T^{ij}_{mnm'n'}(A) = \delta_{mm'} T^{ij}_{mnn'}(A) , \tag{3.24}$$

$$T^{ij}_{-mnn'}(A) = (-1)^{i+j} T^{ij}_{mnn'}(A) . \tag{3.25}$$

Inserting equations (3.24) and (3.25) into equation (3.21), and taking into account the symmetry relation

$$C^{n_1 0}_{n-mn'm} = (-1)^{n+n'+n_1} C^{n_1 0}_{nmn'-m} , \tag{3.26}$$

we obtain the formula

$$T^{ij}_{mnn'} = (-1)^m \sum_{n_1=|n-n'|}^{n+n'} [1 + (-1)^{n+n'+n_1+i+j}] p_{n_1} C^{n_1 0}_{nmn'-m} \sum_{m_1=0}^{M} (-1)^{m_1} (1 - \tfrac{1}{2}\delta_{m_1 0}) C^{n_1 0}_{nm_1n'-m_1} T^{ij}_{m_1nn'}(A) , \tag{3.27}$$

that can be used in practical computations. Also, from equations (3.21) and (3.24)–(3.26), we easily derive a symmetry relation

$$T^{ij}_{-mnn'} = (-1)^{i+j} T^{ij}_{mnn'} . \tag{3.28}$$

Finally, by making use of equations (3.10), (3.28), (A5), (A6), (A8), and the symmetry relation

$$d^n_{-m,-m'}(\theta) = (-1)^{m+m'} d^n_{mm'}(\theta) , \tag{3.29}$$

we obtain

$$\langle F_{11}(\boldsymbol{n}, \boldsymbol{n})\rangle = F_{11}(\theta) = \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \sum_{m=0}^{M} (2-\delta_{m0})\beta_{nn'}\left[T^{11}_{mnn'} \frac{m^2}{\sin^2\theta} d^n_{0m}(\theta)d^{n'}_{0m}(\theta) + T^{12}_{mnn'} \frac{m}{\sin\theta} d^n_{0m}(\theta) \frac{d}{d\theta} d^{n'}_{0m}(\theta) + T^{21}_{mnn'} \frac{d}{d\theta} d^n_{0m}(\theta) \frac{m}{\sin\theta} d^{n'}_{0m}(\theta) + T^{22}_{mnn'} \frac{d}{d\theta} d^n_{0m}(\theta) \frac{d}{d\theta} d^{n'}_{0m}(\theta)\right], \tag{3.30}$$

$$\langle F_{12}(\boldsymbol{n}, \boldsymbol{n})\rangle = \langle F_{21}(\boldsymbol{n}, \boldsymbol{n})\rangle = 0, \tag{3.31}$$

$$\langle F_{22}(\boldsymbol{n}, \boldsymbol{n})\rangle = F_{22}(\theta) = \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \sum_{m=0}^{M} (2-\delta_{m0})\beta_{nn'}\left[T^{11}_{mnn'} \frac{d}{d\theta} d^n_{0m}(\theta) \frac{d}{d\theta} d^{n'}_{0m}(\theta) + T^{12}_{mnn'} \frac{d}{d\theta} d^n_{0m}(\theta) \frac{m}{\sin\theta} d^{n'}_{0m}(\theta) + T^{21}_{mnn'} \frac{m}{\sin\theta} d^n_{0m}(\theta) \frac{d}{d\theta} d^{n'}_{0m}(\theta) + T^{22}_{mnn'} \frac{m^2}{\sin^2\theta} d^n_{0m}(\theta)d^{n'}_{0m}(\theta)\right], \tag{3.32}$$

where

$$\beta_{nn'} = \frac{1}{k} i^{n'-n-1}\left[\frac{(2n+1)(2n'+1)}{n(n+1)n'(n'+1)}\right]^{1/2}. \tag{3.33}$$

Thus, as it follows from equations (2.8) and (3.30)–(3.32), if the local magnetic field is parallel to the z-axis of the laboratory reference frame, then the extinction matrix is given by (cf. Martin 1974)

$$\boldsymbol{K}(\boldsymbol{n}) = \boldsymbol{K}_B(\theta) = -\begin{bmatrix} C_{\text{ext}}(\theta) & C_{\text{pol}}(\theta) & 0 & 0 \\ C_{\text{pol}}(\theta) & C_{\text{ext}}(\theta) & 0 & 0 \\ 0 & 0 & C_{\text{ext}}(\theta) & C_{\text{cpol}}(\theta) \\ 0 & 0 & -C_{\text{cpol}}(\theta) & C_{\text{ext}}(\theta) \end{bmatrix}, \tag{3.34}$$

where C_{ext}, C_{pol}, and C_{cpol} are cross sections for extinction and linear and circular polarization, respectively, given by

$$C_{\text{ext}}(\theta) = \frac{2\pi}{k} \operatorname{Im}\left[F_{11}(\theta) + F_{22}(\theta)\right], \tag{3.35}$$

$$C_{\text{pol}}(\theta) = \frac{2\pi}{k} \operatorname{Im}\left[F_{11}(\theta) - F_{22}(\theta)\right], \tag{3.36}$$

$$C_{\text{cpol}}(\theta) = -\frac{2\pi}{k} \operatorname{Re}\left[F_{11}(\theta) - F_{22}(\theta)\right]. \tag{3.37}$$

b) The General Case

Now we assume that the local magnetic field is not parallel to the z-axis of the laboratory reference frame. Denote by $(\boldsymbol{n}, Z)$ the plane through the vector $\boldsymbol{n}$ and the z-axis of the laboratory reference frame, and by $(\boldsymbol{n}, \boldsymbol{B})$ the plane through the vectors $\boldsymbol{n}$ and $\boldsymbol{B}$. Assume that the extinction matrix $\boldsymbol{K}_B(\theta)$, given by equation (3.34), is known. Let Ω be the angle of the rotation of the plane $(\boldsymbol{n}, Z)$ around the vector $\boldsymbol{n}$ that transforms this plane into the plane $(\boldsymbol{n}, \boldsymbol{B})$. The angle Ω is measured in the clockwise direction, when looking in the direction of light propagation. Then we have (see Martin 1974)

$$\boldsymbol{K}(\boldsymbol{n}) = \boldsymbol{L}(-\Omega)\boldsymbol{K}_B(\theta)\boldsymbol{L}(\Omega), \tag{3.38}$$

where

$$\theta = \cos^{-1}(\boldsymbol{n} \cdot \boldsymbol{B})/|\boldsymbol{B}|, \tag{3.39}$$

and $\boldsymbol{L}(\Omega)$ is the rotation matrix given by

$$\boldsymbol{L}(\Omega) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\Omega & \sin 2\Omega & 0 \\ 0 & -\sin 2\Omega & \cos 2\Omega & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{3.40}$$

IV. DISCUSSION

a) Numerical Considerations

There are seven major numerical steps involved in calculating the orientationally averaged extinction matrix $\boldsymbol{K}(\boldsymbol{n})$ for partially aligned axially symmetric grains.

1. Computation of the T-matrix with respect to the natural reference frame of the scatterer (the matrix $\boldsymbol{T}$[A]).

2. Computation of the expansion coefficients p_n for a given distribution function $p(\beta)$ (eqs. [3.22] and [3.23]).
3. Computation of the Clebsch-Gordan coefficients $C^{n_1 0}_{nmn'-m}$.
4. Computation of the orientationally averaged T-matrix with respect to the reference frame with the z-axis along the local magnetic field (eqs. [3.20] and [3.27]).
5. Computation of the angular functions $(m/\sin\theta)d^n_{0m}(\theta)$ and $(d/d\theta)d^n_{0m}(\theta)$.
6. Computation of the extinction matrix $\boldsymbol{K}_B(\theta)$ (eqs. [3.30]–[3.37]).
7. Computation of the extinction matrix $\boldsymbol{K}(\boldsymbol{n})$ (eqs. [3.38]–[3.40]).

Recurrence formulae for computing the angular functions and the Clebsch-Gordan coefficients are given in Appendices A and B. Formulae for calculating the matrix $\boldsymbol{T}(A)$ for homogeneous axially symmetric particles are given, e.g., by Tsang, Kong, and Shin (1984). Numerical aspects of the T-matrix calculations are discussed by Wiscombe and Mugnai (1986) (note that Wiscombe and Mugnai use another set of vector spherical wave functions in the expansions [3.1] and [3.2]).

b) *Model Distribution Functions*

The size and mineralogical and morphological structure of the interstellar grains as well as the nature of the alignment process are still uncertain and will likely remain so for some years. Because of these uncertainties, the alignment of the grains is not yet well understood. Therefore, at least at a starting point of interpreting the observational data, one has to use an *a priori* chosen simple analytical function instead of the actual distribution function $p(\beta)$. Several model distribution functions are discussed below.

Note that in the Rayleigh limit (the wavelength is much greater than the size of the scattering grains), it is not necessary to know the distribution function $p(\beta)$ itself. Instead, it is sufficient to indicate the parameter

$$\langle\cos^2\beta\rangle = \int_0^\pi d\beta \sin\beta \cos^2\beta p(\beta) , \tag{4.1}$$

$0 \le \langle\cos^2\beta\rangle \le 1$ (see, e.g., Greenberg 1968; Dolginov, Gnedin, and Silant'ev 1979). Therefore, we give the value of this parameter for all the functions considered.

i) *Random Orientation (RO)*

In this case,

$$p(\beta) = \tfrac{1}{2} , \tag{4.2}$$

$$p_0 = 1 , \quad p_n = 0 \quad \text{for} \quad n \ge 1 , \tag{4.3}$$

$$\langle\cos^2\beta\rangle = \tfrac{1}{3} . \tag{4.4}$$

As a result, we have (Mishchenko 1990)

$$T^{ij}_{mnn'} = \frac{1}{2n+1}\delta_{ij}\delta_{nn'}\sum_{m_1=0}^{n}(2-\delta_{m_1 0})T^{ii}_{m_1 nn}(A) , \tag{4.5}$$

$$\boldsymbol{K}(\boldsymbol{n}) = \boldsymbol{K}_B(\theta) = \boldsymbol{K} , \tag{4.6}$$

where

$$K_{pq} = -\delta_{pq}C_{\text{ext}} , \qquad p, q = 1, \dots, 4 , \tag{4.7}$$

$$C_{\text{ext}} = -\frac{2\pi}{k^2}\,\text{Re}\sum_{n=1}^{\infty}\sum_{m=0}^{n}(2-\delta_{m0})[T^{11}_{mnn}(A) + T^{22}_{mnn}(A)] . \tag{4.8}$$

ii) *Perfect Davis-Greenstein Alignment (PDG)*

For flattened grains with a plane of symmetry perpendicular to the axis of symmetry, we have

$$p(\beta) = \delta(\cos\beta - 1) , \tag{4.9}$$

$$p_n = 1 , \qquad n = 0, 1, \dots , \tag{4.10}$$

$$\langle\cos^2\beta\rangle = 1 , \tag{4.11}$$

where $\delta(x)$ is the Dirac delta function. By making use of equations (3.21), (3.24), (4.10), and an equality (see, e.g., Varshalovich, Moskalev, and Khersonskij 1975)

$$\sum_{n_1=|n-n'|}^{n+n'} C^{n_1 0}_{nmn'-m} C^{n_1 0}_{nm_1 n'-m_1} = \delta_{mm_1} , \tag{4.12}$$

we obtain an obvious identity

$$T^{ij}_{mnn'} = T^{ij}_{mnn'}(A) . \tag{4.13}$$

For elongated grains,

$$p(\beta) = \delta(\cos \beta)\,, \tag{4.14}$$

$$p_{2n+1} = 0\,, \qquad p_{2n} = (-1)^n \frac{1 \cdot 3 \ldots (2n-1)}{2 \cdot 4 \ldots 2n}\,, \qquad n = 0, 1, \ldots, \tag{4.15}$$

$$\langle \cos^2 \beta \rangle = 0\,. \tag{4.16}$$

iii) *Imperfect Alignment* (*IA*)

To model imperfect alignment of nonspherical grains, we use the distribution function

$$p(\beta) = \tfrac{1}{2} + \tfrac{5}{2} p_2 P_2(\cos \beta) = \tfrac{1}{2} + \tfrac{5}{4} p_2 (3\cos^2 \beta - 1) \tag{4.17}$$

with

$$\langle \cos^2 \beta \rangle = \tfrac{1}{3} + \tfrac{2}{3} p_2\,. \tag{4.18}$$

For flattened grains,

$$0 \le p_2 \le \tfrac{2}{5}\,, \qquad \tfrac{1}{3} \le \langle \cos^2 \beta \rangle \le \tfrac{3}{5}\,. \tag{4.19}$$

For elongated grains,

$$-\tfrac{1}{5} \le p_2 \le 0\,, \qquad \tfrac{1}{5} \le \langle \cos^2 \beta \rangle \le \tfrac{1}{3}\,. \tag{4.20}$$

c) *Illustrative Numerical Examples*

In Table 1, some illustrative numerical results are given for prolate and oblate spheroidal grains consisting of "astronomical silicate" (Draine and Lee 1984; Draine 1985). The surface of a spheroidal grain in the natural coordinate system A is governed by the equation

$$r(\theta, \varphi) = a(\sin^2 \theta + d^2 \cos^2 \theta)^{-1/2}\,, \qquad d = a/b\,, \tag{4.21}$$

where b is the rotational semiaxis, and a is the horizontal semiaxis of the spheroid.

TABLE 1

EFFICIENCY FACTORS FOR PARTIALLY ALIGNED "ASTRONOMICAL SILICATE" SPHEROIDS

λ (μm)		PDG $\theta = 0°$	PDG $\theta = 30°$	PDG $\theta = 60°$	PDG $\theta = 90°$	IA[a] $\theta = 0°$	IA[a] $\theta = 30°$	IA[a] $\theta = 60°$	IA[a] $\theta = 90°$	RO
					Prolate Spheroids, $d = \frac{1}{2}$					
0.2	$Q_{\rm ext}$	3.11E+0	3.02E+0	2.86E+0	2.62E+0	2.96E+0	2.92E+0	2.83E+0	2.78E+0	2.84E+0
	$Q_{\rm pol}$	0.0	−1.94E−3	−3.04E−2	−5.41E−2	0.0	−4.41E−3	−1.32E−2	−1.77E−2	0.0
	$Q_{\rm cpol}$	0.0	2.35E−4	−5.89E−2	−1.04E−1	0.0	−8.60E−3	−2.58E−2	−3.44E−2	0.0
0.55	$Q_{\rm ext}$	3.30E+0	3.31E+0	3.64E+0	3.91E+0	3.42E+0	3.50E+0	3.64E+0	3.71E+0	3.62E+0
	$Q_{\rm pol}$	0.0	−4.38E−2	−1.66E−1	−2.35E−1	0.0	−2.27E−2	−6.81E−2	−9.08E−2	0.0
	$Q_{\rm cpol}$	0.0	1.00E−2	−6.83E−2	−8.13E−2	0.0	−8.20E−3	−2.46E−2	−3.28E−2	0.0
1.0	$Q_{\rm ext}$	1.14E+0	1.08E+0	9.95E−1	9.58E−1	1.06E+0	1.04E+0	1.01E+0	9.89E−1	1.01E+0
	$Q_{\rm pol}$	0.0	−6.20E−2	−1.55E−1	−1.89E−1	0.0	−1.99E−2	−5.97E−2	−7.97E−2	0.0
	$Q_{\rm cpol}$	0.0	3.09E−2	9.70E−2	1.31E−1	0.0	1.30E−2	3.90E−2	5.20E−2	0.0
5.0	$Q_{\rm ext}$	2.55E−2	2.47E−2	2.29E−2	2.21E−2	2.41E−2	2.38E−2	2.31E−2	2.28E−2	2.32E−2
	$Q_{\rm pol}$	0.0	−8.65E−4	−2.59E−3	−3.44E−3	0.0	−3.44E−4	−1.03E−3	−1.38E−3	0.0
	$Q_{\rm cpol}$	0.0	6.75E−3	2.02E−2	2.68E−2	0.0	2.69E−3	8.06E−3	1.07E−2	0.0
					Oblate Spheroids, $d = 2$					
0.2	$Q_{\rm ext}$	3.00E+0	2.84E+0	2.72E+0	2.24E+0	2.79E+0	2.73E+0	2.60E+0	2.53E+0	2.62E+0
	$Q_{\rm pol}$	0.0	−3.71E−2	−3.51E−2	−2.82E−3	0.0	−4.13E−3	−1.24E−2	−1.65E−2	0.0
	$Q_{\rm cpol}$	0.0	−3.99E−2	−1.64E−1	−1.09E−1	0.0	−1.63E−2	−4.88E−2	−6.50E−2	0.0
0.55	$Q_{\rm ext}$	2.90E+0	2.98E+0	3.80E+0	4.38E+0	3.26E+0	3.43E+0	3.78E+0	3.95E+0	3.72E+0
	$Q_{\rm pol}$	0.0	1.02E−1	−2.63E−1	−5.65E−1	0.0	−4.32E−2	−1.30E−1	−1.73E−1	0.0
	$Q_{\rm cpol}$	0.0	−1.12E−1	−4.03E−1	−5.09E−1	0.0	−5.21E−2	−1.56E−1	−2.08E−1	0.0
1.0	$Q_{\rm ext}$	1.26E+0	1.16E+0	1.01E+0	9.46E−1	1.12E+0	1.09E+0	1.03E+0	9.99E−1	1.04E+0
	$Q_{\rm pol}$	0.0	−1.25E−1	−3.21E−1	−3.94E−1	0.0	−4.14E−2	−1.24E−1	−1.65E−1	0.0
	$Q_{\rm cpol}$	0.0	1.10E−1	3.16E−1	4.11E−1	0.0	4.17E−2	1.25E−1	1.67E−1	0.0
5.0	$Q_{\rm ext}$	2.76E−2	2.60E−2	2.29E−2	2.13E−2	2.51E−2	2.44E−2	2.32E−2	2.26E−2	2.34E−2
	$Q_{\rm pol}$	0.0	−1.59E−3	−4.75E−3	−6.32E−3	0.0	−6.32E−4	−1.90E−3	−2.53E−3	0.0
	$Q_{\rm cpol}$	0.0	1.36E−2	4.06E−2	5.41E−2	0.0	5.41E−3	1.62E−2	2.16E−2	0.0

[a] For prolate spheroids, $\langle \cos^2 \beta \rangle = \frac{1}{5}$; for oblate spheroids, $\langle \cos^2 \beta \rangle = \frac{3}{5}$.

For convenience, we tabulate efficiency factors instead of the cross sections. Efficiency factors for extinction and linear and circular polarization, respectively, are given by

$$Q_{\rm ext}(\theta) = C_{\rm ext}(\theta)/(\pi r_{\rm ev}^2)\,, \tag{4.22}$$

$$Q_{\rm pol}(\theta) = C_{\rm pol}(\theta)/(\pi r_{\rm ev}^2)\,, \tag{4.23}$$

$$Q_{\rm cpol}(\theta) = C_{\rm cpol}(\theta)/(\pi r_{\rm ev}^2)\,, \tag{4.24}$$

where $r_{\rm ev}$ is the radius of the equal-volume sphere. For spheroids,

$$r_{\rm ev} = ad^{-1/3}\,. \tag{4.25}$$

All the numerical data in Table 1 are given for $r_{\rm ev} = 0.2\ \mu$m.

d) *Numerical Checks*

To examine the accuracy of our computer code, several test calculations have been performed.

1. The T-matrix computations for "partially aligned" homogeneous spheres were compared with the corresponding Mie calculations. In the "averaging" process, the distribution functions (4.2), (4.9), (4.14), and (4.17) were used.
2. The result of using the uniform distribution function (4.2) was compared with that of using the formulae (4.5)–(4.8).
3. To calculate the "averaged" T-matrix for perfectly aligned grains, the distribution function (4.9) was used, and then the "averaged" T-matrix was compared with the original matrix $T(A)$ (see eq. [4.13]).
4. The results of the T-matrix computations for partially aligned "Rayleigh" spheroids ($\lambda \gg r_{\rm ev}$) were compared with those obtained by use of the corresponding asymptotic analytical formulae (see § V).
5. The reciprocity relation (2.9) was used for checking purposes. For the matrix $\boldsymbol{K}_B(\theta)$, the relation gives

$$\boldsymbol{K}_B(\pi - \theta) = \boldsymbol{K}_B(\theta)\,. \tag{4.26}$$

It should be noted here that if (1) the scattering grain has a plane of symmetry perpendicular to the axis of symmetry or (2) the distribution function $p(\beta)$ obeys the symmetry relation

$$p(\pi - \beta) = p(\beta)\,, \tag{4.27}$$

then the equality (4.26) follows also from the ensemble symmetry with respect to the plane XOY of the laboratory coordinate system. Nevertheless, if both conditions (1) and (2) are violated, then the symmetry relation (4.26) is of less trivial nature.

6. The T-matrix computations were compared with those of Asano (1983) for "horizontally oriented" oblate and prolate spheroids. In other words, the distribution functions (4.9) and (4.14), respectively, were used in the averaging process. Asano presents graphically a nondimensional extinction cross section $k^2C_{\rm ext}$ for oblate spheroids with $a/b = 5$ and a refractive index $m_r = 1.290 + 0.0945i$, and prolate spheroids with $a/b = \frac{1}{3}$ and refractive indices $m_r = 1.31$ and $m_r = 1.290 + 0.0945i$. For checking purposes, we used Asano's results for $kb = 8$, 16 (prolate spheroids, $m_r = 1.31$), $kb = 10$ (prolate spheroids, $m_r = 1.290 + 0.0945i$), and $ka = 10$ (oblate spheroids, $m_r = 1.290 + 0.0945i$).

In all the cases considered, an excellent agreement was found.

e) *Timing Tests*

Extensive timing tests have shown that, as a rule, the averaging process (see § IV*a*) (steps [2]–[7]) requires only a small fraction of the time that is necessary for calculating the T-matrix with respect to the natural reference frame (step [1]). As an example, in Table 2 we give (in seconds) the computational times for calculating the matrices $T(A)$ (step [1]), $\langle T\rangle_{\rm PDG}$, and $\langle T\rangle_{\rm IA}$ (steps [2]–[4]) for prolate spheroids with $d = \frac{1}{2}$ and $m_r = 2.259 + 0.5296i$. The wavelength is 0.2 μm. In the computations, a computer ES 1061 was used. The parameters $n_{\rm max}$ and $m_{\rm max}$ are the highest n- and m-values, respectively, used in the expansions (3.1) and (3.2), and N_G is the number of Gaussian quadrature points used in the numerical calculation of surface integrals (see Wiscombe and Mugnai 1986, §§ V and VI). The given values of the parameters are chosen to ensure 0.1% accuracy of the computations. Also, in Table 2 we indicate the time for computing the extinction matrix $\boldsymbol{K}_B$ for one value of the zenith angle θ (steps [5] and [6]).

V. THE RANGE OF VALIDITY OF THE RAYLEIGH APPROXIMATION

If the size of scattering grains is much smaller than the wavelength, then the Rayleigh approximation is frequently used (see, e.g., van de Hulst 1957; Greenberg 1968; Dolginov, Gnedin, and Silant'ev 1979; Bohren and Huffman 1983; Draine and Lee 1984; Kleinman and Senior 1986). However, the range of validity of the Rayleigh approximation in computing the full extinction matrix for partially aligned nonspherical grains was not examined by means of rigorous calculations. It was studied only for the extinction

TABLE 2

TIMING TEST

$r_{\rm ev}$ (μm)	$n_{\rm max}$	$m_{\rm max}$	N_G	t_A	$t_{\rm PDG}$	$t_{\rm IA}$	t_K
0.2	22	8	50	84.23	21.18	0.68	0.49
0.1	13	5	30	13.44	2.98	0.21	0.12
0.04	8	3	20	2.74	0.53	0.07	0.03

efficiency factor of absorbing ($\mathrm{Im}\, m_r \neq 0$) and dielectric ($\mathrm{Im}\, m_r = 0$) spheres (see Ku and Felske 1984, and references therein), and randomly oriented absorbing spheroids (Mishchenko 1990). In particular, Mishchenko has found that the range does not depend upon the asphericity of grains, and depends only upon their refractive index. In other words, whatever the aspect ratio of randomly oriented spheriods is, a condition ensuring a given (say, 1%) accuracy of the Rayleigh-limit calculations of the extinction efficiency factor can be formulated as

$$x \leq x_{\max}\,, \tag{5.1}$$

where x is the equal-volume–sphere size parameter, given by

$$x = 2\pi r_{ev}/\lambda\,, \tag{5.2}$$

and the parameter $x_{\max}$ is equal to that from the corresponding condition for the equal-volume sphere of the same refractive index (Ku and Felske 1984).

In the low-frequency limit, the efficiency factors for absorbing partially aligned spheroidal grains are given by (see, e.g., Dolginov, Gnedin, and Silant'ev 1979)

$$Q^R_{\mathrm{ext}}(\theta) = x\ \mathrm{Im}\ [q_1(\theta) + q_2(\theta)]\,, \tag{5.3}$$

$$Q^R_{\mathrm{pol}}(\theta) = x\ \mathrm{Im}\ [q_1(\theta) - q_2(\theta)]\,, \tag{5.4}$$

$$Q^R_{\mathrm{cpol}}(\theta) = -x\ \mathrm{Re}\ [q_1(\theta) - q_2(\theta)]\,, \tag{5.5}$$

where

$$q_1(\theta) = \tfrac{1}{3}\{[(1 + \langle\cos^2\beta\rangle)\beta_x + (1 - \langle\cos^2\beta\rangle)\beta_z]\cos^2\theta + 2[(1 - \langle\cos^2\beta\rangle)\beta_x + \langle\cos^2\beta\rangle\beta_z]\sin^2\theta\}\,, \tag{5.6}$$

$$q_2(\theta) = \tfrac{1}{3}[(1 + \langle\cos^2\beta\rangle)\beta_x + (1 - \langle\cos^2\beta\rangle)\beta_z]\,, \tag{5.7}$$

$$\beta_j = \frac{m_r^2 - 1}{1 + (m_r^2 - 1)L_j}\,, \qquad j = x, z\,. \tag{5.8}$$

For prolate spheroids ($d < 1$),

$$L_z = \frac{1 - e^2}{2e^3}\left[\ln\frac{1 + e}{1 - e} - 2e\right], \qquad e^2 = 1 - d^2\,. \tag{5.9}$$

For oblate spheroids ($d > 1$),

$$L_z = \frac{1 + e^2}{e^3}(e - \tan^{-1} e)\,, \qquad e^2 = d^2 - 1\,. \tag{5.10}$$

The quantity L_x is given by

$$L_x = (1 - L_z)/2\,. \tag{5.11}$$

To examine the accuracy of the Rayleigh approximation, we used the T-matrix approach and equations (5.3)–(5.11) to compute the efficiency factors Q and Q^R for partially aligned spheroids in the range $1.1 \leq \mathrm{Re}\, m_r \leq 10$, $0.001 \leq \mathrm{Im}\, m_r \leq 10$, $\frac{1}{5} \leq d \leq 5$. Extensive computations have shown that, at least in the range considered, the condition (5.1) can be used also in calculating the full extinction matrix for partially aligned absorbing spheroids. As an example, in Table 3 the T-matrix and the Rayleigh-limit computations are compared for the refractive indices $m_r = 1.7 + 0.03i$ and $m_r = 2.5 + i$; the scattering grains are oblate spheroids with $a/b = 5$. The analytical criteria of Ku and Felske (1984) ensuring 1% accuracy in calculating the Mie extinction efficiency are

$$x_{\max} = 0.0691|m_r|^{-11/8} \quad \text{for} \quad \mathrm{Im}\, m_r \geq 0.001\,, \tag{5.12}$$

$$x_{\max} = 0.238|m_r|^{-5/3} \quad \text{for} \quad \mathrm{Im}\, m_r \geq 0.1\,. \tag{5.13}$$

By using these criteria, we find that $x_{\max} = 0.03331$ for $m_r = 1.7 + 0.03i$, and $x_{\max} = 0.04567$ for $m_r = 2.5 + i$. The corresponding Mie efficiency factors are $Q_{\mathrm{ext}} = 0.00171$, $Q^R_{\mathrm{ext}} = 0.00170$ for $m_r = 1.7 + 0.03i$, and $Q_{\mathrm{ext}} = 0.0355$, $Q^R_{\mathrm{ext}} = 0.0353$ for $m_r = 2.5 + i$. It is seen from Table 3 that the criteria (5.12) and (5.13) ensure 1% accuracy for all the efficiency factors for partially aligned spheroids of even sufficiently high aspect ratio.

VI. CONCLUSIONS

The main results of this study are summarized in the following three points.

1. The problem of model theoretical calculation of the interstellar extinction and linear and circular polarization due to nonspherical grains, partially aligned in a magnetic field, is outlined. The Waterman's T-matrix approach is used to develop an efficient method to calculate the extinction matrix averaged over orientations of a nonspherical grain. Instead of evaluating numerically the integral in a definition

$$K(n) = \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma P(\alpha, \beta, \gamma)K(n; \alpha, \beta, \gamma)\,,$$

TABLE 3

EFFICIENCY FACTORS FOR SMALL PARTIALLY ALIGNED SPHEROIDS

Parameter	PDG $\theta = 0°$	PDG $\theta = 30°$	PDG $\theta = 60°$	PDG $\theta = 90°$	IA[a] $\theta = 0°$	IA[a] $\theta = 30°$	IA[a] $\theta = 60°$	IA[a] $\theta = 90°$	RO
				$m_r = 1.7 + 0.03i$, $x = 0.03331$					
Q_{ext}	2.97E−3	2.70E−3	2.15E−3	1.87E−3	2.53E−3	2.42E−3	2.20E−3	2.09E−3	2.24E−3
Q_{pol}	0.0	−2.74E−4	−8.23E−4	−1.10E−3	0.0	−1.10E−4	−3.29E−4	−4.39E−4	0.0
Q_{cpol}	0.0	4.15E−3	1.25E−2	1.66E−2	0.0	1.66E−3	4.98E−3	6.64E−3	0.0
Q^R_{ext}	2.97E−3	2.69E−3	2.14E−3	1.87E−3	2.53E−3	2.42E−3	2.20E−3	2.09E−3	2.24E−3
Q^R_{pol}	0.0	−2.74E−4	−8.22E−4	−1.10E−3	0.0	−1.10E−4	−3.29E−4	−4.38E−4	0.0
Q^R_{cpol}	0.0	4.15E−3	1.24E−2	1.66E−2	0.0	1.66E−3	4.98E−3	6.64E−3	0.0
				$m_r = 2.5 + i$, $x = 0.04567$					
Q_{ext}	1.12E−1	9.91E−2	7.36E−2	6.08E−2	9.15E−2	8.64E−2	7.61E−2	7.10E−2	7.78E−2
Q_{pol}	0.0	−1.28E−2	−3.84E−2	−5.12E−2	0.0	−5.12E−3	−1.54E−2	−2.05E−2	0.0
Q_{cpol}	0.0	1.81E−2	5.42E−2	7.22E−2	0.0	7.22E−3	2.17E−2	2.89E−2	0.0
Q^R_{ext}	1.11E−1	9.88E−2	7.33E−2	6.06E−2	9.11E−2	8.60E−2	7.58E−2	7.07E−2	7.75E−2
Q^R_{pol}	0.0	−1.27E−2	−3.82E−2	−5.09E−2	0.0	−5.09E−3	−1.53E−2	−2.04E−2	0.0
Q^R_{cpol}	0.0	1.80E−2	5.41E−2	7.21E−2	0.0	7.21E−3	2.16E−2	2.88E−2	0.0

[a] $\langle \cos^2 \beta \rangle = \frac{3}{5}$.

where $\boldsymbol{K}(\boldsymbol{n}; \alpha, \beta, \gamma)$ is the extinction matrix of a particle with orientation specified by the Eulerian angles α, β, and γ, and $P(\alpha, \beta, \gamma)$ is a probability density function, we first analytically average the T-matrix in the coordinate system with the z-axis along the local magnetic field (eqs. [3.20] and [3.21]), and then use equations (2.8), (3.10), and (3.38) to calculate the orientationally averaged extinction matrix $\boldsymbol{K}(\boldsymbol{n})$ with respect to a given laboratory reference frame.[2]

In principle, the proposed method can be applied to particles of arbitrary size, morphology, and composition. Nevertheless, like the T-matrix approach itself, the method is of practical use only for axially symmetric homogeneous and composite isotropic particles of size not too large as compared to the wavelength.

2. Numerical aspects of the proposed averaging method are described in detail. Several analytical functions to model axially symmetric distributions of scattering grains over orientations are briefly discussed. Some illustrative numerical results are given for partially aligned spheroidal grains consisting of "astronomical silicate." The accuracy of the method is examined, and results of timing tests are presented. It is found that in calculating the orientationally averaged extinction matrix, the most part of the computational time is spent for calculating the T-matrix of the grain with respect to the natural reference frame. In other words, the averaging step in calculating the orientationally averaged extinction matrix for partially aligned grains requires only a very small additional computational time as compared to the calculations for perfectly aligned particles.

3. The range of validity of the Rayleigh approximation in computing the orientationally averaged extinction matrix for partially aligned absorbing spheroidal grains is examined. It is found that, irrespective of the asphericity of grains and the degree of their alignment, as well as the direction of light propagation, the condition ensuring a given accuracy of the Rayleigh approximation can be formulated in terms of the equal-volume–sphere size parameter and is exactly the same as for the equal-volume sphere of the same refractive index.

APPENDIX A

WIGNER D-FUNCTIONS AND VECTOR SPHERICAL WAVES

The Wigner D-functions and the vector spherical wave functions are given by

$$D^n_{mm'}(\alpha, \beta, \gamma) = \exp(-im\alpha) d^n_{mm'}(\beta) \exp(-im'\gamma) , \tag{A1}$$

$$\boldsymbol{M}_{mn}(kr) = (-1)^m d_n h^{(1)}_n(kr) \boldsymbol{C}_{mn}(\theta) \exp(im\varphi) , \tag{A2}$$

$$\boldsymbol{N}_{mn}(kr) = (-1)^m d_n \left\{ \frac{n(n+1)}{kr} h^{(1)}_n(kr) \boldsymbol{P}_{mn}(\theta) + \frac{1}{kr} [kr h^{(1)}_n(kr)]' \boldsymbol{B}_{mn}(\theta) \right\} \exp(im\varphi) , \tag{A3}$$

[2] We note here that the idea of taking an ensemble average analytically was recently used by Singham, Singham, and Salzman (1986) and Schiffer (1989) in calculating the orientationally averaged scattering matrix for randomly oriented nonspherical particles. As a basis, Singham, Singham, and Salzman used the discrete-dipole method, whereas Schiffer used the so-called perturbation approach.

where

$$d^n_{mm'}(\beta) = [(n+m)!(n-m)!(n+m')!(n-m')!]^{1/2} \sum_j (-1)^{j+n-m'} \frac{(\cos \beta/2)^{m+m'+2j}(\sin \beta/2)^{2n-m-m'-2j}}{j!(n-m-j)!(n-m'-j)!(m+m'+j)!}, \quad n \geq \max(|m|, |m'|), \tag{A4}$$

$$\boldsymbol{B}_{mn}(\theta) = \hat{\boldsymbol{\theta}} \frac{d}{d\theta} d^n_{0m}(\theta) + \hat{\boldsymbol{\varphi}} \frac{im}{\sin \theta} d^n_{0m}(\theta), \tag{A5}$$

$$\boldsymbol{C}_{mn}(\theta) = \hat{\boldsymbol{\theta}} \frac{im}{\sin \theta} d^n_{0m}(\theta) - \hat{\boldsymbol{\varphi}} \frac{d}{d\theta} d^n_{0m}(\theta), \tag{A6}$$

$$\boldsymbol{P}_{mn}(\theta) = \hat{\boldsymbol{r}} d^n_{0m}(\theta), \tag{A7}$$

$$d_n = \left[\frac{2n+1}{4\pi n(n+1)}\right]^{1/2}. \tag{A8}$$

The summation in equation (A4) is such that $j \geq 0$, and all the factorials in the summation are nonnegative. The expressions for the functions Rg $\boldsymbol{M}_{mn}$ and Rg $\boldsymbol{N}_{mn}$ can be obtained from equations (A2) and (A3) by replacing spherical Hankel functions $h^{(1)}_n$ by spherical Bessel functions j_n. The functions $d^n_{mm'}$ can be expressed in Jacobi polynomials as follows:

$$d^n_{mm'}(\beta) = e_{mm'} \left[\frac{s!(s+a+b)!}{(s+a)!(s+b)!}\right]^{1/2} \left(\cos \frac{\beta}{2}\right)^b \left(\sin \frac{\beta}{2}\right)^a P^{(a,b)}_s(\cos \beta), \tag{A9}$$

where

$$a = |m - m'|, \quad b = |m + m'|, \quad s = n - (a+b)/2,$$

$$e_{mm'} = \begin{cases} 1 & \text{for} \quad m' \geq m, \\ (-1)^{m'-m} & \text{for} \quad m' < m. \end{cases}$$

Also we have

$$d^n_{00}(\beta) = P_n(\cos \beta), \tag{A10}$$

$$d^n_{0m}(\beta) = (-1)^m \left[\frac{(n-m)!}{(n+m)!}\right]^{1/2} P^m_n(\cos \beta), \tag{A11}$$

$$d^n_{mm'}(\beta) = i^{m'-m} P^n_{mm'}(\cos \beta), \tag{A12}$$

where $P_n(x)$ are Legendre polynomials given by

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n, \tag{A13}$$

$P^m_n(x)$ are associated Legendre functions given by

$$P^m_n(x) = \frac{(-1)^m}{2^n n!} (1 - x^2)^{m/2} \frac{d^{n+m}}{dx^{n+m}} (x^2 - 1)^n, \tag{A14}$$

and $P^n_{mm'}(x)$ are generalized spherical functions (Gel'fand, Minlos, and Shapiro 1963).

For computing the angular functions appearing in equations (3.30) and (3.32), the following recurrence relations can be used (Varshalovich, Moskalev, and Khersonskij 1975):

$$d^{n+1}_{0m}(\beta) = [(2n+1) \cos \beta \, d^n_{0m}(\beta) - (n^2 - m^2)^{1/2} d^{n-1}_{0m}(\beta)][(n+1)^2 - m^2]^{-1/2}, \tag{A15}$$

$$d^{m-1}_{0m}(\beta) = 0, \qquad d^m_{0m}(\beta) = A_m (1 - \cos^2 \beta)^{m/2}, \tag{A16}$$

$$A_0 = 1, \qquad A_m = A_{m-1} \left[\frac{2m-1}{2m}\right]^{1/2}, \tag{A17}$$

$$\frac{d}{d\beta} d^n_{0m}(\beta) = \frac{m \cos \beta}{\sin \beta} d^n_{0m}(\beta) - [(n-m)(n+m+1)]^{1/2} d^n_{0m+1}(\beta) \tag{A18}$$

$$= -\frac{m\cos\beta}{\sin\beta}\, d^n_{0m}(\beta) + [(n+m)(n-m+1)]^{1/2}\, d^n_{0m-1}(\beta)\,. \tag{A19}$$

Also, one should take into account symmetry relations

$$d^n_{0m}(\pi-\beta) = (-1)^{n+m} d^n_{0m}(\beta)\,, \tag{A20}$$

$$\frac{d}{d\beta'}\, d^n_{0m}(\beta')\Big|_{\beta'=\pi-\beta} = (-1)^{n+m+1}\frac{d}{d\beta'}\, d^n_{0m}(\beta')\Big|_{\beta'=\beta}\,. \tag{A21}$$

Finally, one easily obtains for $m \geq 0$

$$\frac{m\, d^n_{0m}(\beta)}{\sin\beta}\Big|_{\beta=0} = \frac{d}{d\beta}\, d^n_{0m}(\beta)\Big|_{\beta=0} = \frac{1}{2}\,\delta_{m1}[n(n+1)]^{1/2}\,. \tag{A22}$$

APPENDIX B

CLEBSCH-GORDAN COEFFICIENTS

For calculating the Clebsch-Gordan coefficients appearing in equation (3.27), one can use the recurrence relation

$$C^{n_1 0}_{nmn'-m} = \left[\frac{4(2n_1+1)(2n_1-1)}{(n-n'+n_1)(-n+n'+n_1)(n+n'-n_1+1)(n+n'+n+1)}\right]^{1/2} \times \left\{mC^{n_1-1\,0}_{nmn'-m} - \left[\frac{(-n+n'+n_1-1)(n-n'+n_1-1)(n+n'-n_1+2)(n+n'+n_1)}{4(2n_1-3)(2n_1-1)}\right]^{1/2} C^{n_1-2\,0}_{nmn'-m}\right\} \tag{B1}$$

with $n \geq n'$ and starting values

$$C^{n-n'-1\,0}_{nmn'-m} = 0\,, \tag{B2}$$

$$C^{n-n'\,0}_{nmn'-m} = C_{nn'm}\,, \tag{B3}$$

where

$$C_{n'n'm} = (-1)^{n'+m}(2n'+1)^{-1/2}\,, \tag{B4}$$

$$C_{n+1,n',m} = C_{nn'm}\left[\frac{(n+m+1)(n-m+1)(2n-2n'+3)}{(n+1)(2n+3)(n-n'+1)}\right]^{1/2}. \tag{B5}$$

(cf. Varshalovich, Moskalev, and Khersonskij 1975, eqs. [8.5.1], [8.5.13], and [8.6.27]). For $n < n'$, the symmetry relation

$$C^{n_1 0}_{nmn'-m} = C^{n_1 0}_{n'mn-m} \tag{B6}$$

is used.

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